

Application Brief AB-059

ASTROMID-18, GLUCONIC ACID, & OTHER AQUEOUS-BASED LIBRARY COMPOUNDS

Recently, we have received many questions from TravelIR HCl™ and HazMatID™ customers as to why Astromid-18™, Gluconic Acid and other such products appear in their library hit lists when certain samples are analyzed. This Technical Note addresses these questions and how to understand such results.

Recall that when a sample is analyzed with a TravelIR HCl or a HazMatID, an infrared (IR) spectrum is obtained that represents the chemical bonds constituting the molecules in the sample. This spectrum is characteristic of the sample and is often called a "molecular fingerprint." Unknown samples are identified by recording their IR fingerprints and comparing them to libraries of known reference fingerprints. The analysis result is a list of library compounds whose spectra "look most like" the sample spectrum, and a number is given on a scale from 0 - 1 (the "similarity" value S) that indicates how well the sample and each library hit match.

When mixture sample is analyzed, the measured IR spectrum represents the spectra of all the individual components, weighted by their relative concentrations in the mixture. Water is a unique chemical because it has a strong IR absorbance, and when it's in a mixture, water contributes a lot to the measured spectrum, as shown in Figure 1. Any sample that contains a fair amount of water will have a tendency to match library spectra of the same constitution. Astromid-18 and Gluconic Acid are examples of mixture

samples containing significant amounts of water. Astromid-18 is the tradename of a commercial product containing a surfactant, which is a type of chemical that helps polar and non-polar chemicals mix together. The surfactant itself is an organic compound, and it is mixed with water in the formulated product. Gluconic acid is another organic compound that is used as a chelating agent, which is a type of chemical that grabs onto components such as metal ions dissolved in water. Gluconic acid is commercially available for industrial applications as a 50% solution in water.

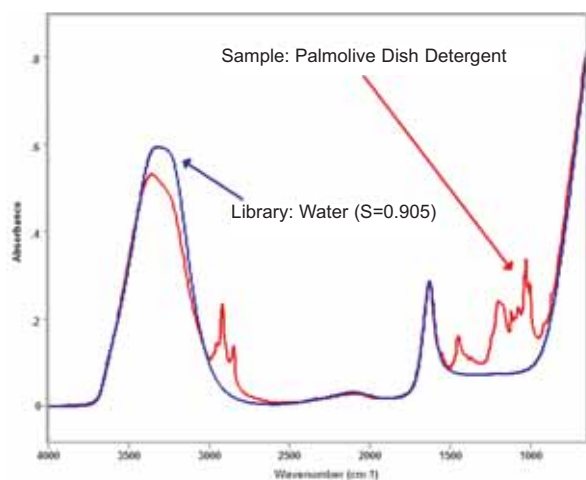


Figure 1. Substances that contain a lot of water, such as dish detergent, produce IR spectra that have a strong water component and tend to match well with other aqueous substances, as shown in Figure 2.

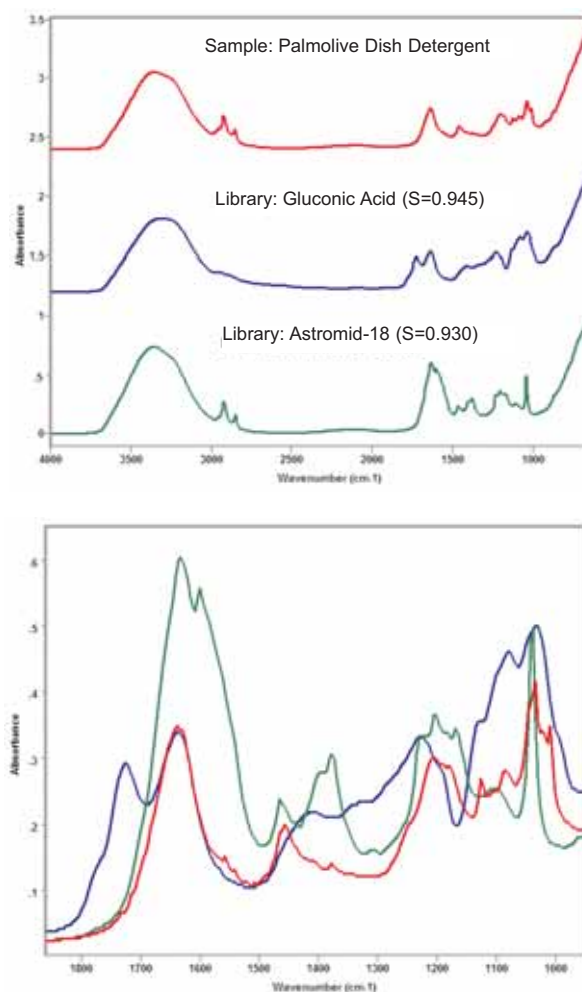


Figure 2. TOP: A library search of a dish detergent spectrum (red) results in matches with Gluconic Acid (blue) and Astromid-18 (green), though neither of the matches is good enough to render a positive identity. **BOTTOM:** A closer look from 1800 - 1000 cm^{-1} at the spectra shows that none of them are identical, suggesting that the organic components in the water-based samples are all different.

Going by our above discussion of mixture samples, it follows that any sample consisting of organic chemicals mixed with water can produce matches with Astromid-18 and Gluconic Acid. Examples include alcoholic beverages, cleaning solutions, and contaminated water. Figure 2 illustrates such an analysis, in which a liquid detergent (basically a surfactant and water) was analyzed on a HazMatID. The top two matches were Gluconic Acid and Astromid-18, and each had relatively high similarity values (0.90) because all of these substances contain water and some organic material. However, the expanded view of all three spectra indicates that neither Gluconic Acid nor Astromid-18 is truly a good match for the liquid detergent, since each substance has unique peaks and none of the spectra overlap very well. One would conclude from this analysis that the sample (assuming it was an "unknown") is a water-based substance containing some other organic material, but it is not consistent with Gluconic Acid, Astromid-18, or any of the library spectra available for the analysis.

It cannot be understated that the TravellIR HCI and the HazMatID do not identify substances - the user does. These instruments simply provide valuable information that facilitates the process. Consequently, they should always be used in conjunction with other instruments and meters to obtain a full understanding of the sample identity and potential hazards. You can learn more about IR analysis, dealing with mixture samples, and other TravellIR HCI and HazMatID topics at our Educational Corner at www.hazmatid.com.